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Estimation of acoustic impedance of binary liquid system from 288.15 to 318.15K by associated and non-associated process

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Abstract

In the present study acoustic impedance (Z) was computed for weakly interacting liquid mixture of 1-butanol and dodecane over the entire concentration range and atmospheric pressure from 288.15-318.15K. Flory's statistical liquid state model based on non-association process and models based on association process such as Ramaswamy- Anbananthan (RS) and Gilinsky have been applied for the computation of aforesaid acoustical parameters and compared with the experimental work of J. Peleterio. McAllister multibody interaction model based on Eyring's theory of absolute reaction rate was used to correlate the experimental results in terms in terms of numerical coefficients and standard deviation. Theoretical results calculated from association process deals a good agreement with experimental results in comparison to non-association process.

Keywords: Flory' statistical model; Ramaswamy; ultrasonic speed; acoustic impedance.

Introduction

In past few years ultrasonic parameters have become a subject of deep interest for researchers[1-4] in the analysis of various thermodynamic properties and the molecular interactions present between the components of liquid mixtures. Theoretical interpretation of these parameters plays a significant role in absence of experimental data for the prediction of molecular interaction and other physicochemical properties. In the continuation of our previously published work[5] this paper is concerned with the estimation of acoustic impedance for the aforesaid liquid mixture from 288.15-318. 15K. Flory's model[6-10] based on non-association process, Ramaswamy [11] model and a model corrected by Glinski[12] based on association process were used to compute the ultrasonic parameters of binary liquid mixture over the entire concentration range and atmospheric pressure at different temperatures. Association constant (K_{as}) and adjustable parameters (Z_{ab}) are two important criteria for the computation of various thermodynamic properties for Ramaswamy and Glinski models. The handling procedure of these two liquid state models was almost similar. While statistical model of Flory assumes the additivity of liquids. Theoretical values were compared and tested with measured values of J. Peleterio[13]. McAllister[14] model based on Eyring's theory of absolute reaction rate was used to correlate the experimental results in terms in terms of numerical coefficients and standard deviation. The main aim of this work to study the molecular interactions of binary liquid mixture based on the calculation of acoustic impedance at various temperatures by aforementioned liquid state models and to test their applicability.

Modeling

Flory model: Flory[6-10] proposed a most famous liquid state model based on the additivity of liquids. Ultrasonic speed can be calculated by Auerbach equation because Flory theory has no direct relation with ultrasonic speed

$$U_{Flory} = \left[\frac{\sigma}{6.3 \times 10^{-4} \rho_{Mix}}\right]^{2/3} \quad (1)$$

Where: σ and ρ_{Mix} are surface tension and density of binary liquid mixture respectively.

Ramaswamy model: Ramaswamy model[11] based on the linear relation of acoustic impedance with the mole fraction of liquid components.

$$Z_{RS} = [X_1 Z_1 + X_2 Z_2 + X_{12} Z_{12}]\theta \quad (2)$$

Where: θ is adjustable parameter which depend on the temperature.

Glinski model: Glinski[12] model based on association process assume additivity with the volume fraction (Φ) of components of liquids.

$$Z_{Glinski} = \frac{Z_1 Z_{12} Z_2}{\emptyset_1 Z_2 Z_{12} + \emptyset_2 Z_1 Z_{12} + \emptyset_{12} Z_1 Z_2} \quad (3)$$

Where: $\emptyset_1$, $\emptyset_2$ and $\emptyset_{12}$ are volume fraction of pure liquid components and their associates respectively.

McAllister model: McAllister model[14] based on the assumption of Eyring's theory of absolute rate. Which is used to correlate the various physicochemical properties with measured values.

McAllister-3- body:

$$\ln Z = x_1^3 \ln Z_1 + 3x_1^2 x_2 \ln Z_{A_0} + 3x_1 {x_2}^2 \ln Z_{A_1} + x_2^3 \ln Z_2 - \ln[x_1 + x_2 M_2/M_1] + 3x_1^2 x_2 \ln[(2 + M_2/M_1)/3] + 3x_1 x_2^2 \ln[(1 + 2\,M_2/M_1)/3] + x_2^3 \ln[M_2/M_1] \quad (4)$$

McAllister-4-body:

$$\ln Z = x_1^4 \ln Z_1 + 4x_1^3 x_2 \ln Z_{A_0} + 6x_1^2 x_2^2 \ln Z_{A_1} + 4x_1 x_2^2 \ln Z_{A_2} + x_2^4 \ln Z_2 - \ln[(x_1 + x_2 M_2/M_1)] + 4x_1^3 x_2 \ln[(3 + M_2/M_1)/4] + 6x_1^2 x_2^2 \ln[(1 + M_2/M_1)/2] + 4x_1 x_2^3 \ln[(1 + 3M_2/M_1)/4] + x_2^4 \ln(M_2/M_1) \quad (5)$$

Where: A_0, A_1 and A_2 are adjustable parameters. Which were calculated by least square method. M_1 and M_2 are molecular weight of pure liquids.

Acoustic impedance: Acoustic impedance (Z) can be calculated by following relation:

$$Z = (U) \times \left(\rho_{Mix}\right) \quad (6)$$

Where: U is ultrasonic speed of binary liquid mixture calculated by liquid state models.

Results and discussion

Table-1 represents experimental and theoretical acoustic impedance computed from various liquid state models along with their percentage deviation from 288.15-318.15K. Table-2 represents the parameters and standard deviation (σ_Z) calculated for McAllister-3-body and McAllister-4-body interaction models from 288.15-318. 15K.

$$\sigma_Z = \left[\sum_{i=1}^{n} \frac{(Z_{Exp} - Z_{Cal})}{n-p}\right]^{1/2} \quad (7)$$

Where n is number of experimental points and p is number of adjustable parameters. Standard deviation for McAllister-3-body lies in the range ($0.00032<\sigma_Z<0.00034$), whereas in case of McAllister-4-body model its value lies in range ($0.00023<\sigma_Z<0.00030$), which indicate fair agreement with experimental findings. Average absolute % deviation (AAPD) computed from Flory, Ramaswamy and Glinski models for acoustic impedance along with their association constant and adjustable parameters at various temperatures are presented in Table-3. A close observation of Table-1 reveals that density of binary mixture and acoustic impedance increases with increase in mole fraction of 1-butanol except few points. Which indicate that molecular interaction increases with increase in the concentration of 1-butanol. Density and acoustic impedance of binary liquid mixture decreases with increase in temperature was due to the breaking of intermolecular force of attraction between the components of binary liquid mixture.

Deviation in acoustic impedance with mole fraction of aforesaid binary mixture at different temperatures are presented in Figure-1. Negative deviation in acoustic impedance was observed for all the liquid state models except Flory model which show positive deviation at 298.15K and 308.15K. The trend was almost similar for all the liquid state models. Negative deviation in acoustic impedance confirms that the system under consideration was highly compressed due to dipole- induced dipole interaction.

A perusal of Table-2 clearly indicates that McAllister-4-body model deals a fair agreement of correlation with experimental findings in comparison to McAllister-3-body model. Standard deviation of McAllister-4-body model decreases with increase in temperature while in case of McAllister-3-body model standard deviation increases. A careful observation of Table-3 indicate that AAPD of Flory model varies from (0.2856-2.0709), Ramaswamy (1.2759-1.6187) and Glinski model (1.5343-2.5524) which indicate that Ramaswamy model based on association process deals a fair agreement with experimental results in comparison to Flory and Glinski model. Increasing order of AAPD is as follows: Ramaswamy < Flory < Glinski. AAPD for McAllister-3 and 4-body interaction model varies from (0.0219-0.2238) and (0.0185-0.0205). Which clearly indicate that McAllister-4-body model consist of high degree of accuracy in the correlation with experimental findings at different temperatures in comparison to McAllister-3-body model.

Conclusion

From the above discussion it can be concluded that density of binary liquid mixture plays a significant role in the determination of acoustic impedance. In the present investigation non-linear variation in acoustic impedance with mole fraction confirm the intermolecular interaction between the binary components.

Acoustic impedance decreases with increase in temperature predict the dissociation of molecular interaction between like and unlike liquid components. McAllister-4 body model based on least square method correlates the experimental findings with high degree of accuracy. Ramaswamy model based on association process deals a fair agreement with experimental findings in comparison to others.

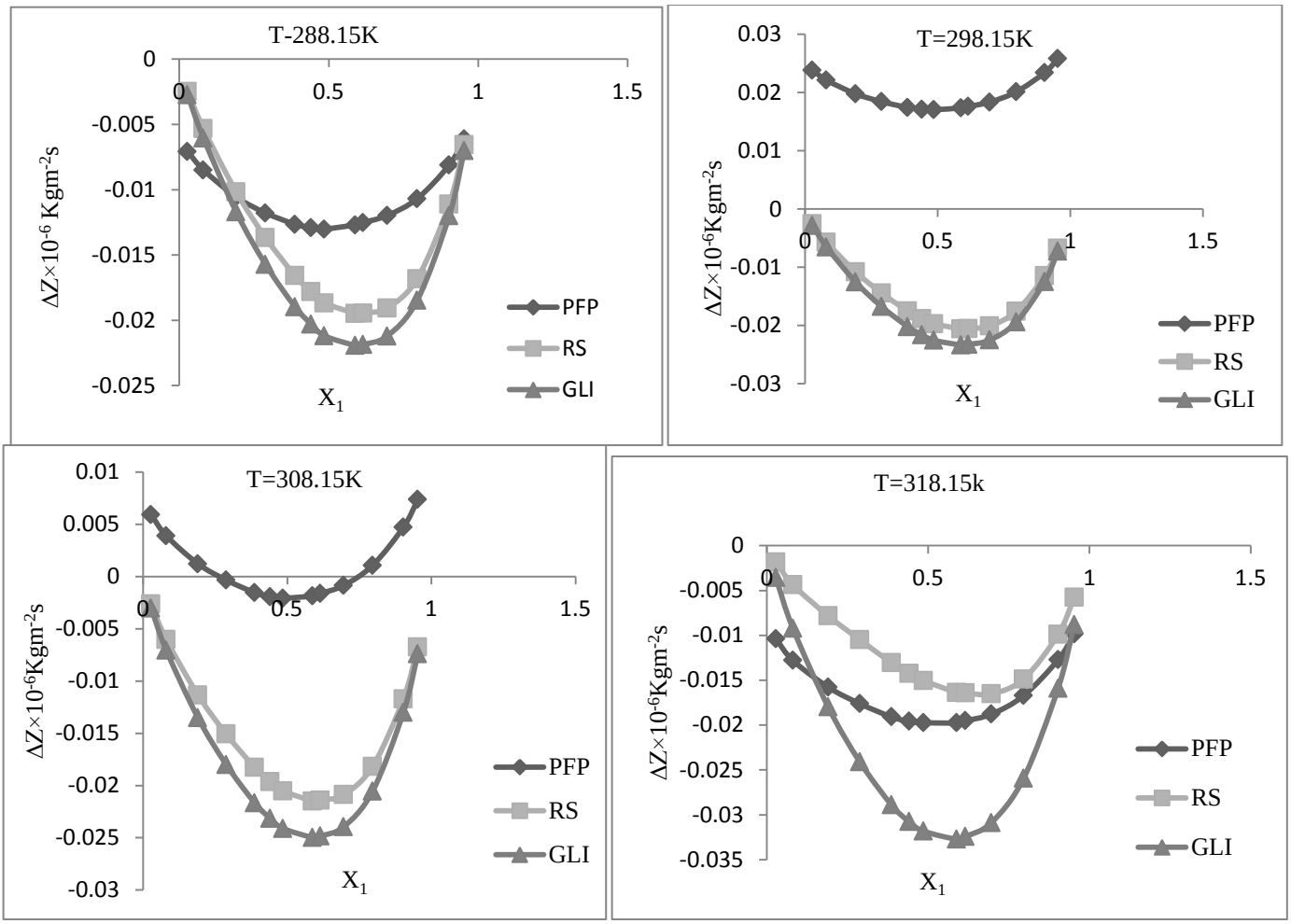

Figure-1: Plot of deviation in acoustic impedance of 1-butannol+dodecane from 288.15-318.

Table-1: Experimental and Theoretical acoustic impedance from 288.15-318.15K.

X_1	ρ^{Mix}	Z_{exp} X 10^{-6}	Z_{PFP} X 10^{-6}	Z_{RS} X 10^{-6}	Z_{GLI} X 10^{-6}	% ΔPFP	% ΔRS	% ΔGLI
T=288.15K								
0.02749	752.75	0.9897	0.9967	0.9921	0.9924	-0.71	-0.25	-0.28
0.08048	753.82	0.9889	0.9974	0.9942	0.9950	-0.86	-0.54	-0.61
0.19017	756.5	0.9885	0.9990	0.9987	1.0002	-1.07	-1.03	-1.18
0.28812	759.47	0.9891	1.0009	1.0027	1.0048	-1.19	-1.38	-1.59
0.38654	762.98	0.9904	1.0030	1.0070	1.0094	-1.28	-1.67	-1.91
0.44097	765.23	0.9916	1.0045	1.0094	1.0118	-1.30	-1.80	-2.05
0.4853	767.14	0.9927	1.0057	1.0113	1.0139	-1.31	-1.88	-2.13
0.58849	772.65	0.9965	1.0092	1.0160	1.0185	-1.27	-1.95	-2.20
0.61515	774.27	0.9978	1.0103	1.0172	1.0197	-1.25	-1.95	-2.19

0.69605	779.63	1.0020	1.0140	1.0210	1.0232	-1.19	-1.90	-2.12
0.79594	787.76	1.0090	1.0197	1.0258	1.0275	-1.06	-1.67	-1.83
0.90295	799.12	1.0200	1.0281	1.0311	1.0320	-0.79	-1.09	-1.18
0.95321	805.7	1.0271	1.0332	1.0336	1.0341	-0.59	-0.64	-0.68
T=298.15K								
0.02749	745.49	0.9510	0.9272	0.9536	0.9539	2.51	-0.27	-0.30
0.08048	746.51	0.9500	0.9279	0.9557	0.9565	2.33	-0.60	-0.68
0.19017	749.12	0.9494	0.9296	0.9602	0.9619	2.09	-1.14	-1.32
0.28812	752.04	0.9500	0.9315	0.9644	0.9667	1.94	-1.52	-1.76
0.38654	755.51	0.9512	0.9338	0.9687	0.9714	1.83	-1.84	-2.12
0.44097	757.73	0.9524	0.9352	0.9712	0.9740	1.80	-1.98	-2.27
0.4853	759.62	0.9535	0.9364	0.9732	0.9760	1.79	-2.07	-2.36
0.58849	765.09	0.9574	0.9401	0.9780	0.9808	1.82	-2.15	-2.44
0.61515	766.72	0.9588	0.9411	0.9793	0.9820	1.84	-2.14	-2.42
0.69605	772.04	0.9631	0.9448	0.9832	0.9856	1.91	-2.08	-2.34
0.79594	780.2	0.9706	0.9505	0.9881	0.9900	2.08	-1.81	-2.00
0.90295	791.57	0.9822	0.9587	0.9936	0.9946	2.39	-1.16	-1.27
0.95321	798.15	0.9895	0.9637	0.9962	0.9967	2.61	-0.68	-0.73
T=308.15K								
0.02749	738.18	0.9134	0.9074	0.9160	0.9164	0.65	-0.29	-0.33
0.08048	739.13	0.9121	0.9082	0.9181	0.9191	0.43	-0.66	-0.77
0.19017	741.67	0.9113	0.9101	0.9226	0.9248	0.13	-1.24	-1.48
0.28812	744.51	0.9117	0.9121	0.9268	0.9297	-0.04	-1.65	-1.97
0.38654	747.93	0.9129	0.9144	0.9312	0.9346	-0.17	-2.00	-2.37
0.44097	750.12	0.9140	0.9160	0.9337	0.9372	-0.21	-2.15	-2.53
0.4853	752.00	0.9152	0.9173	0.9357	0.9393	-0.23	-2.24	-2.63
0.58849	757.40	0.9192	0.9210	0.9406	0.9441	-0.20	-2.34	-2.72
0.61515	759.03	0.9205	0.9222	0.9419	0.9454	-0.18	-2.33	-2.70
0.69605	764.36	0.9251	0.9259	0.9460	0.9490	-0.09	-2.26	-2.59
0.79594	772.5	0.9329	0.9318	0.9511	0.9534	0.11	-1.95	-2.20

0.90295	783.88	0.9450	0.9403	0.9567	0.9580	0.50	-1.24	-1.37
0.95321	790.48	0.9527	0.9454	0.9595	0.9601	0.77	-0.71	-0.78
T=318.15K								
0.02749	730.8	0.8768	0.8871	0.8786	0.8803	-1.18	-0.21	-0.41
0.08048	731.65	0.8751	0.8879	0.8795	0.8843	-1.46	-0.50	-1.05
0.19017	734.12	0.8742	0.8899	0.8820	0.8922	-1.80	-0.90	-2.06
0.28812	736.86	0.8744	0.8920	0.8849	0.8985	-2.01	-1.20	-2.76
0.38654	740.2	0.8755	0.8945	0.8885	0.9044	-2.18	-1.49	-3.30
0.44097	742.36	0.8765	0.8961	0.8908	0.9073	-2.23	-1.63	-3.51
0.4853	744.23	0.8778	0.8975	0.8928	0.9096	-2.25	-1.71	-3.62
0.58849	749.54	0.8816	0.9014	0.8980	0.9144	-2.24	-1.86	-3.71
0.61515	751.18	0.8831	0.9026	0.8995	0.9155	-2.21	-1.86	-3.67
0.69605	756.46	0.8877	0.9065	0.9042	0.9186	-2.12	-1.86	-3.48
0.79594	764.59	0.8958	0.9125	0.9107	0.9218	-1.87	-1.66	-2.90
0.90295	775.98	0.9085	0.9212	0.9184	0.9244	-1.40	-1.09	-1.75
0.95321	782.6	0.9165	0.9264	0.9223	0.9253	-1.08	-0.63	-0.96

Table-2: Parameters of Correlation models from 288.15-318.15K.

T/K	McAllister-3-body			McAllister-4-body			
	A_0	A_1	σ(z)	A_0	A_1	A_2	σ(z)
288.15	0.5419	0.7378	0.00032	1.0308	1.0165	0.9936	0.00030
298.15	0.5201	0.7082	0.00033	0.9902	0.9761	0.9538	0.00028
308.15	0.4989	0.6792	0.00034	0.9504	0.9367	0.9148	0.00027
318.15	0.4778	0.6513	0.00032	0.9113	0.8979	0.8773	0.00023

Table-3: Average absolute % deviation of acoustic impedance from 288.15-318.15K.

T/K	K_{as}	Z_{ab} x10^6	Average absolute % deviation				
			Z_{PFP}	Z_{RS}	Z_{GLI}	Z_{Mc3}	Z_{Mc4}
288.15	0.006	1.00	1.0683	1.3643	1.5343	0.0221	0.0217
298.15	0.007	0.96	2.0709	1.4940	1.6933	0.0219	0.0216
308.15	0.009	0.95	0.2856	1.6187	1.8811	0.0237	0.0205
318.15	0.04	0.91	1.8491	1.2759	2.5524	0.0238	0.0185

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